LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060948.D
Acq On : 18 Apr 2024 23:21
Operator : MA/JU
Sample : P2124-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-131-SB02

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060948.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.158	24	29	38	rVB	92716	134957	3.27%	0.639%
2	3.675	110	117	130	rBV	120332	185888	4.51%	0.880%
3	5.525	425	432	443	rBV	1000842	1537830	37.28%	7.282%
4	7.106	692	701	711	rBV	1100610	1820870	44.14%	8.622%
5	7.940	836	843	849	rBV	194398	313592	7.60%	1.485%
6	9.092	1029	1039	1047	rBV	630221	1088546	26.39%	5.155%
7	10.731	1310	1318	1326	rBV	237315	426712	10.34%	2.021%
8	11.466	1438	1443	1449	rBV2	37221	61676	1.49%	0.292%
9	13.193	1729	1737	1749	rBV	1563681	2420030	58.66%	11.460%
10	14.562	1961	1970	1981	rBV	459305	726146	17.60%	3.439%
11	14.791	1999	2009	2016	rBV2	59328	133953	3.25%	0.634%
12	16.054	2217	2224	2231	rBV	1855920	2860430	69.33%	13.545%
13	17.312	2431	2438	2445	rBV	696102	1048952	25.43%	4.967%
14	18.222	2586	2593	2601	rBV	457739	664760	16.11%	3.148%
15	19.368	2786	2788	2798	rVB6	24475	45340	1.10%	0.215%
16	19.491	2805	2809	2818	rBV	114230	169217	4.10%	0.801%
17	19.938	2879	2885	2894	rVB	3127359	4125529	100.00%	19.536%
18	21.242	3102	3107	3119	rBV2	311674	541767	13.13%	2.565%
19	21.571	3156	3163	3169	rBV	713346	1172604	28.42%	5.553%
20	22.406	3300	3305	3314	rVB3	63415	144668	3.51%	0.685%
21	23.258	3444	3450	3459	rBV	40378	76647	1.86%	0.363%
22	23.863	3548	3553	3559	rBV3	30223	56940	1.38%	0.270%
23	24.691	3683	3694	3704	rBV	484303	1289621	31.26%	6.107%
24	25.902	3893	3900	3908	rVB5	24810	71197	1.73%	0.337%

Sum of corrected areas: 21117872

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
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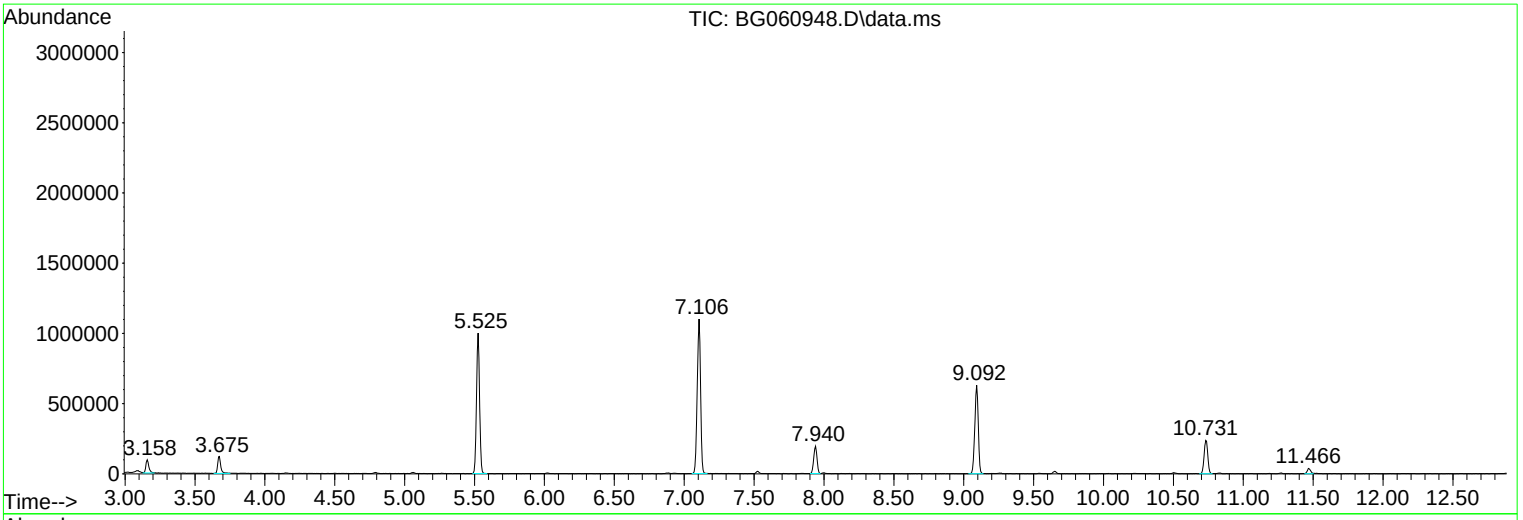
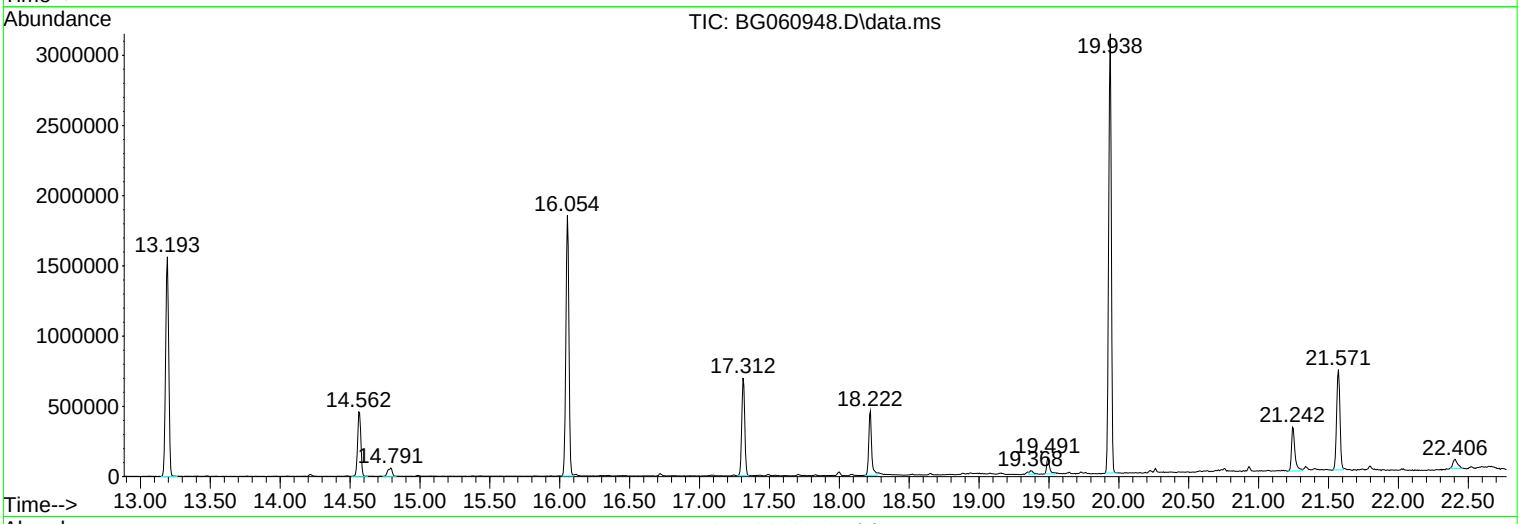
Operator : MA/JU
Sample : P2124-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

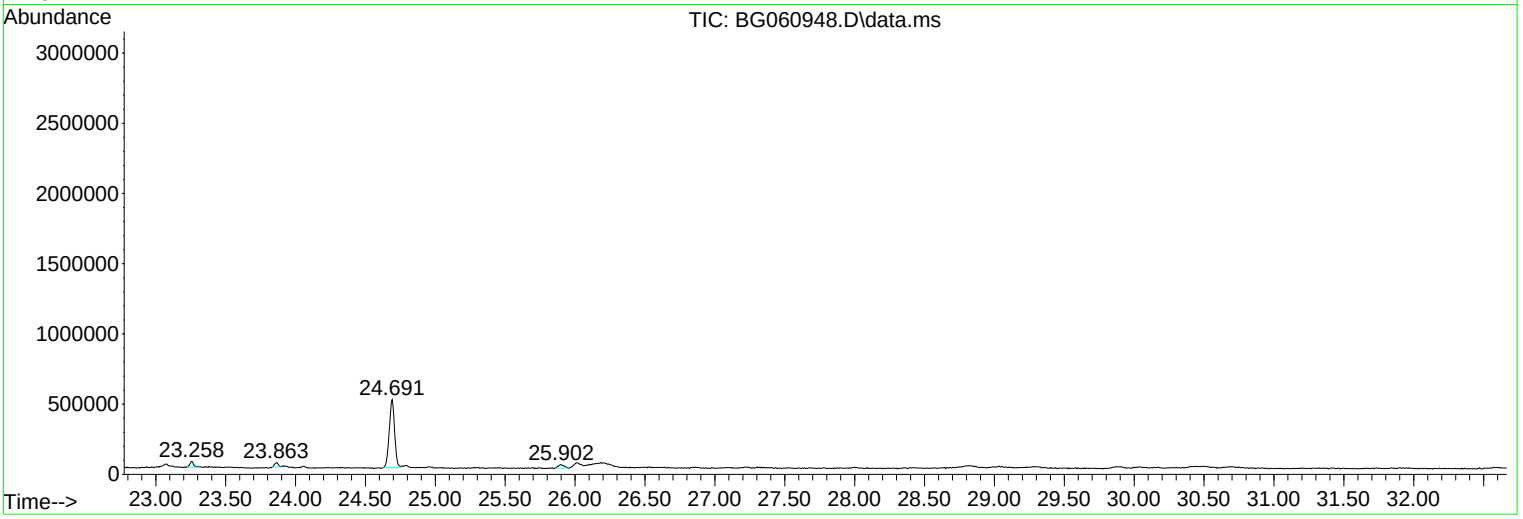
Instrument :
BNA_G
ClientSampleId :
B-131-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Data File : BG060948.D
Acq On : 18 Apr 2024 23:21
Operator : MA/JU
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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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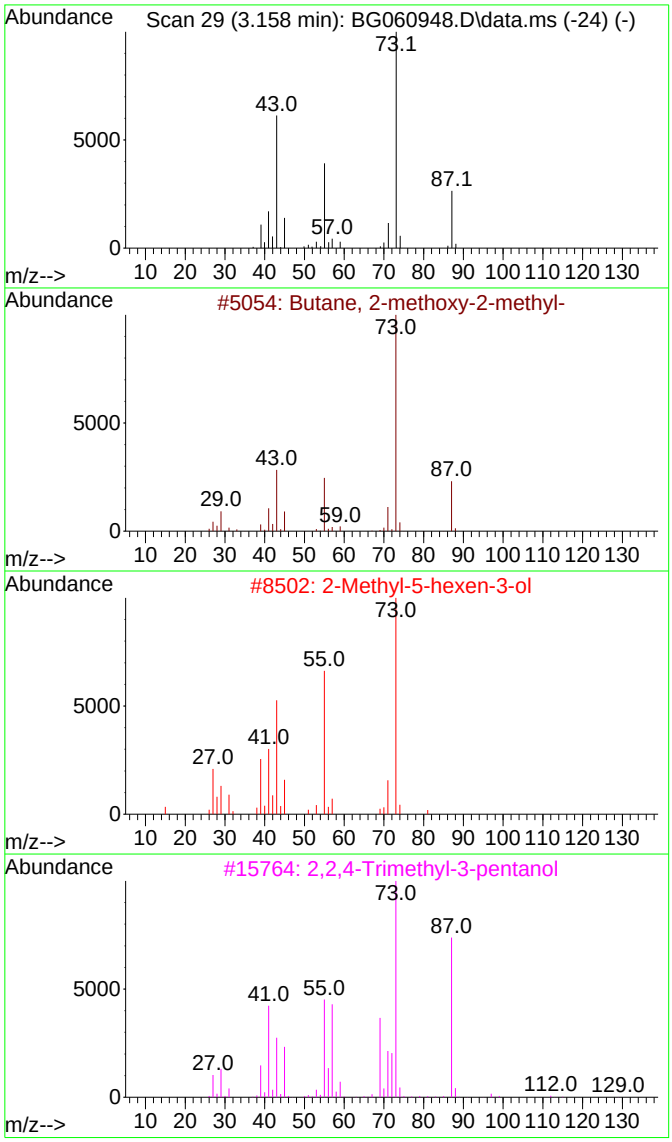
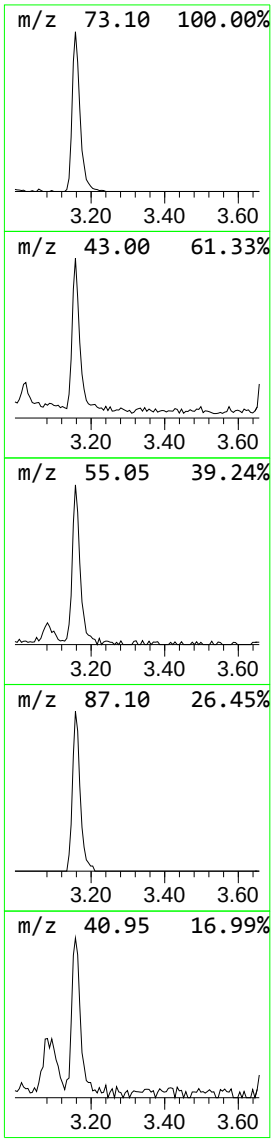
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.158	8.61 ng	134957	1,4-Dichlorobenzene-d4	7.940

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	50
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28
5	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	23





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Data File : BG060948.D
Acq On : 18 Apr 2024 23:21
Operator : MA/JU
Sample : P2124-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-131-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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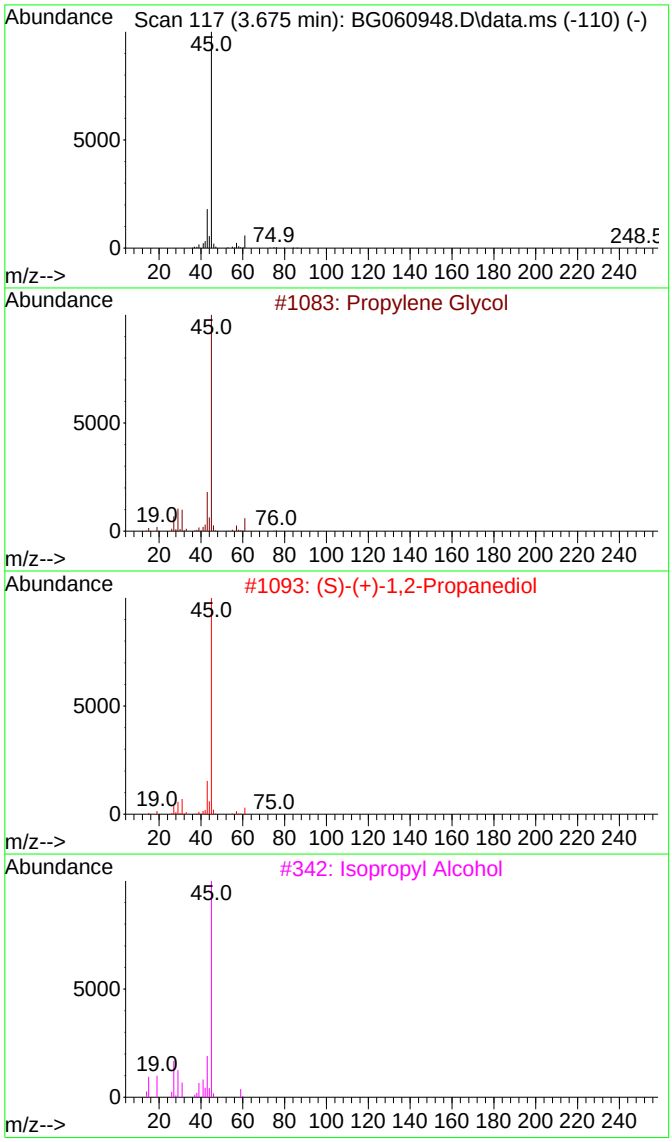
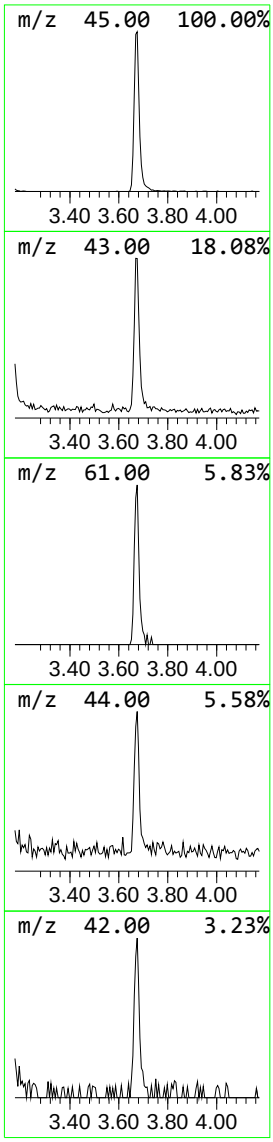
Peak Number 2 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.675	11.86 ng	185888	1,4-Dichlorobenzene-d4	7.940

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	32





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Data File : BG060948.D
Acq On : 18 Apr 2024 23:21
Operator : MA/JU
Sample : P2124-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-131-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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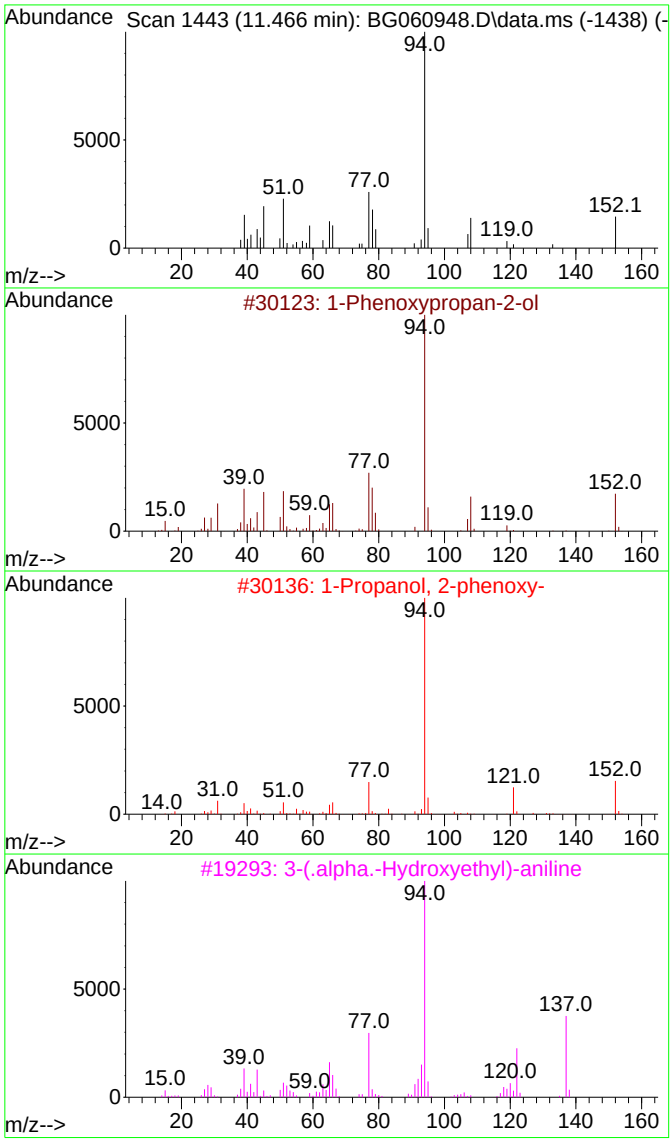
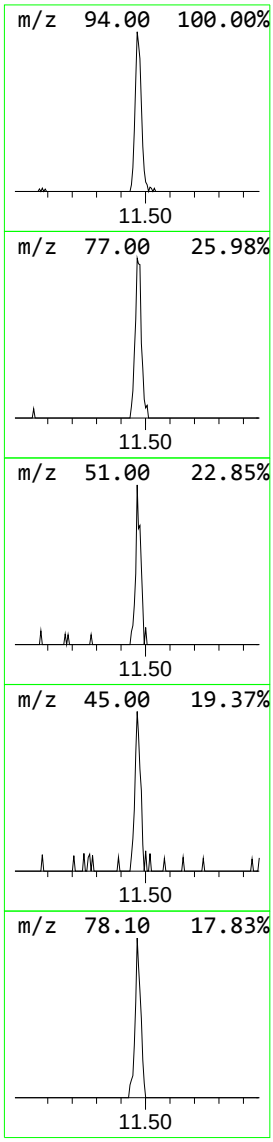
Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.466	2.89 ng	61676	Naphthalene-d8	10.731

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	53
3	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	47
4	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	47
5	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	38





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Data File : BG060948.D
Acq On : 18 Apr 2024 23:21
Operator : MA/JU
Sample : P2124-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-131-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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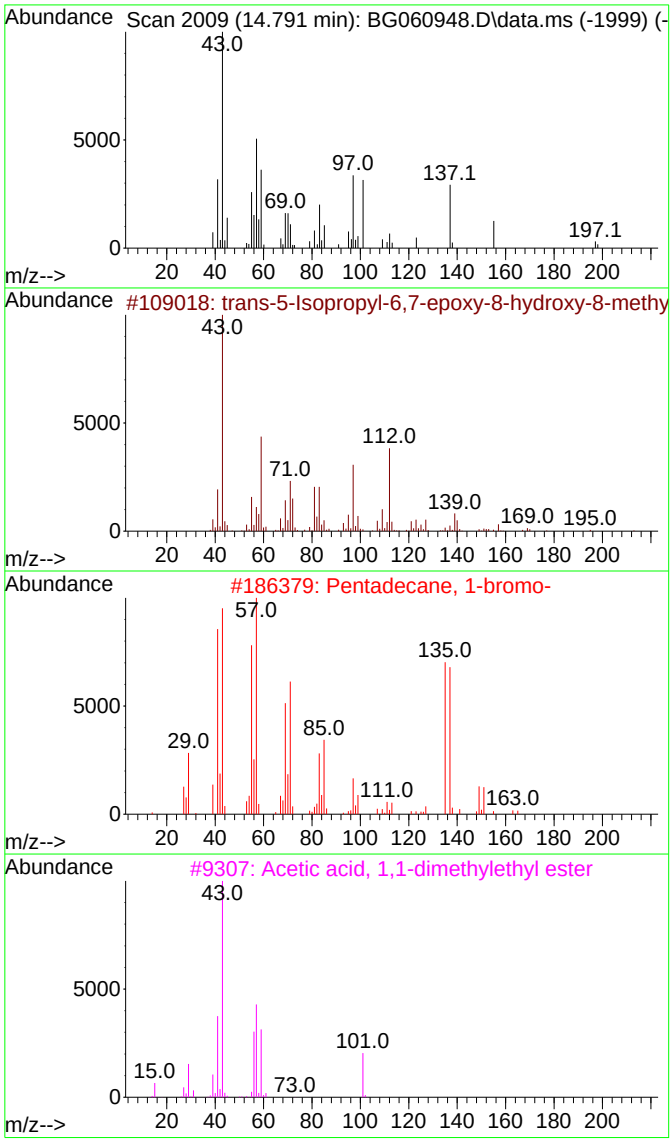
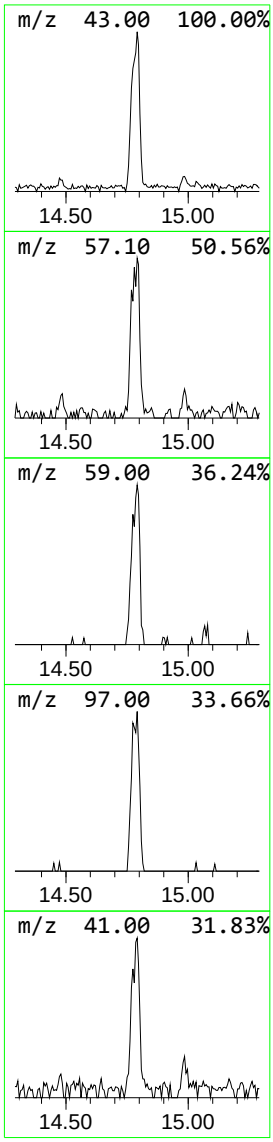
Peak Number 4 unknown14.791 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.791	3.69 ng	133953	Acenaphthene-d10	14.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	32
2	Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	14
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
4	Bromoacetic acid, decyl ester	278	C12H23BrO2	005436-93-1	10
5	Tridecane, 1-bromo-	262	C13H27Br	000765-09-3	10





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Operator : MA/JU
Sample : P2124-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-131-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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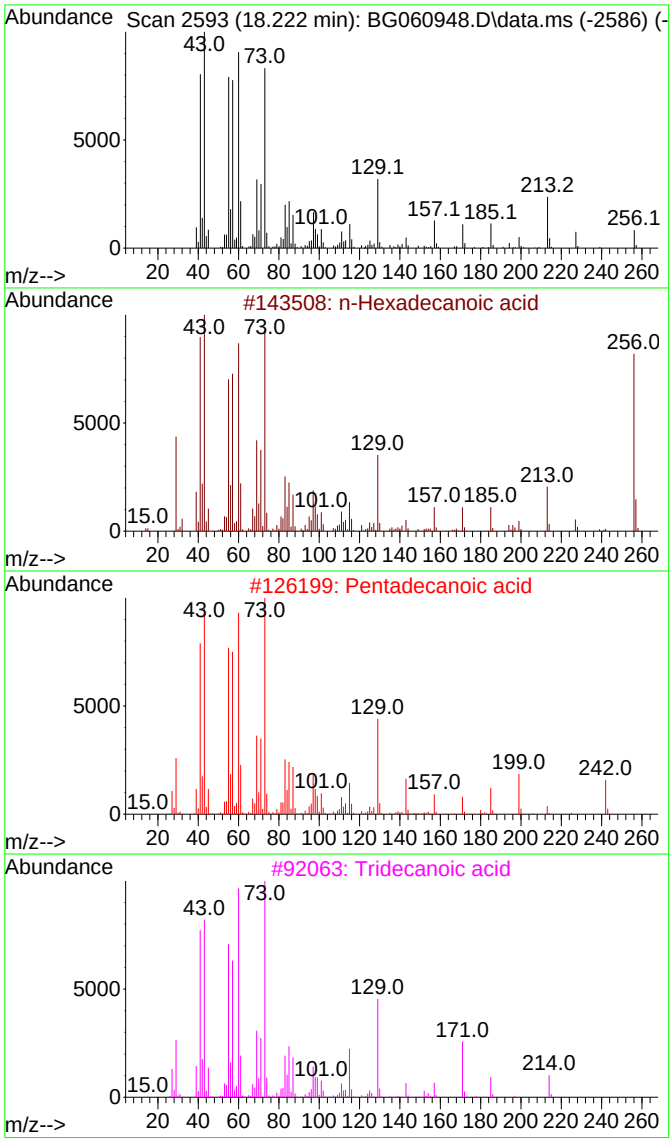
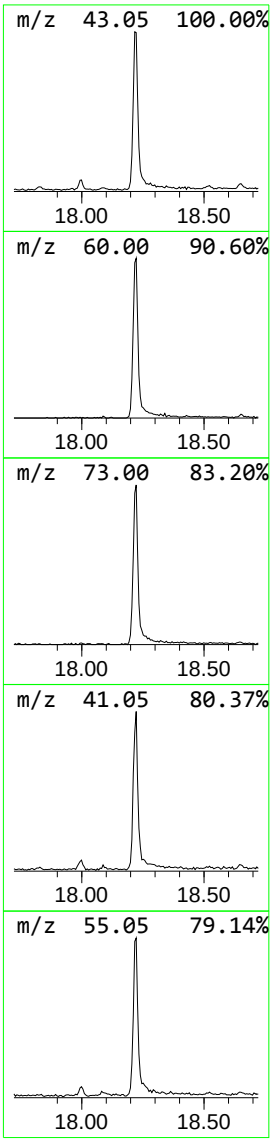
Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	12.67 ng	664760	Phenanthrene-d10	17.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060948.D
Acq On : 18 Apr 2024 23:21
Operator : MA/JU
Sample : P2124-02
Misc :
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Instrument :
BNA_G
ClientSampleId :
B-131-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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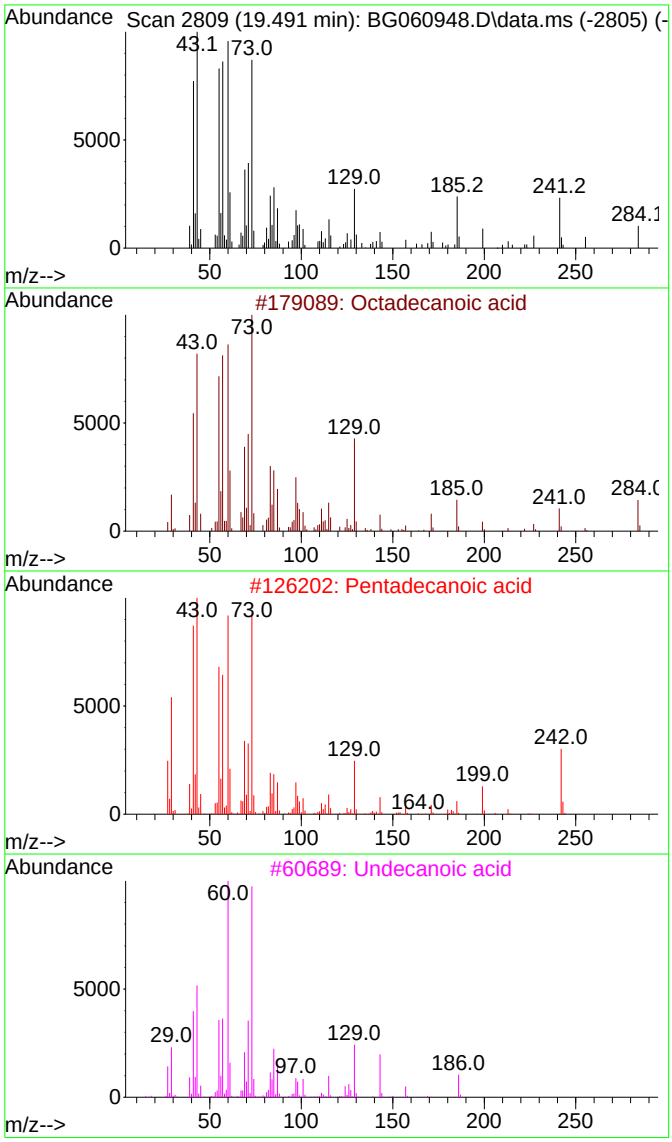
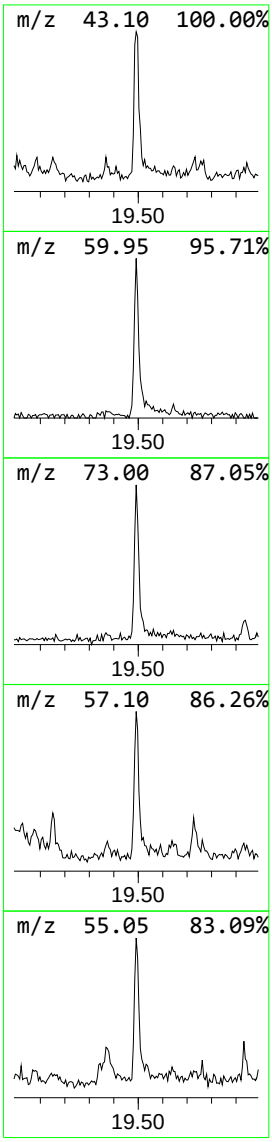
Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.491	2.89 ng	169217	Chrysene-d12	21.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	95
3	Undecanoic acid	186	C11H22O2	000112-37-8	70
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Data File : BG060948.D
Acq On : 18 Apr 2024 23:21
Operator : MA/JU
Sample : P2124-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-131-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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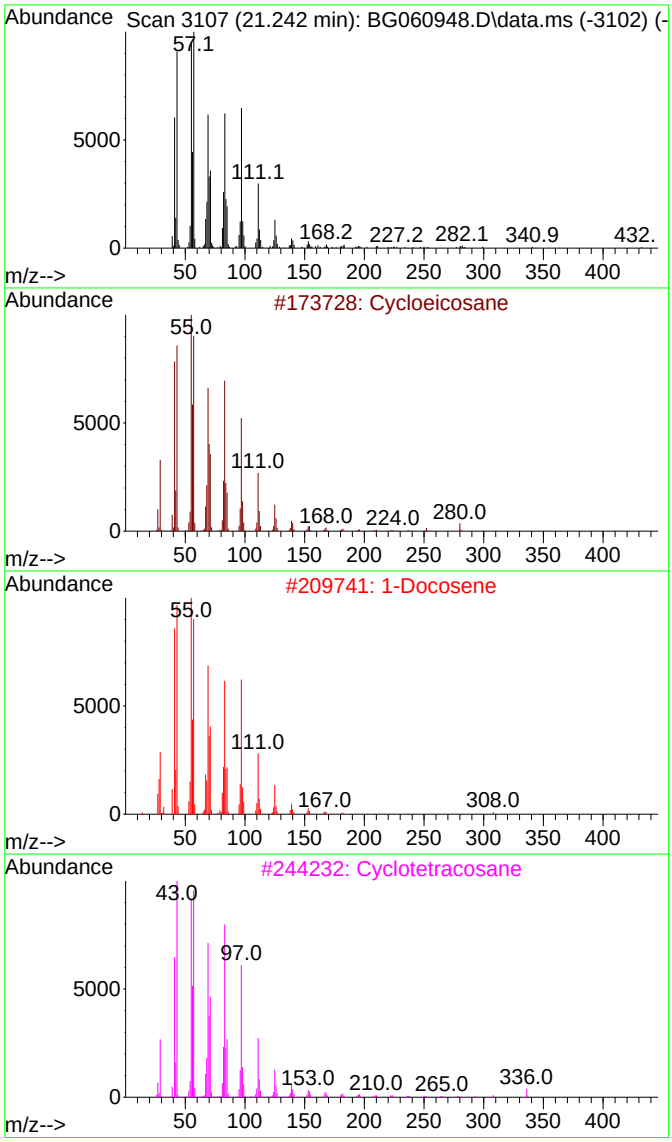
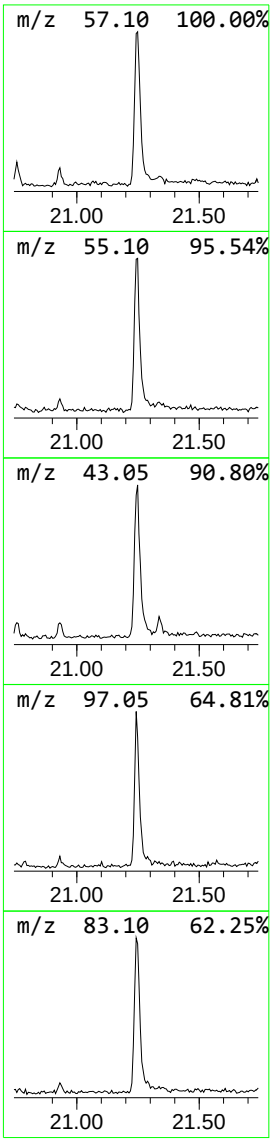
Peak Number 7 Cycloeicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.242	9.24 ng	541767	Chrysene-d12	21.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	Cyclotetracosane	336	C24H48	000297-03-0	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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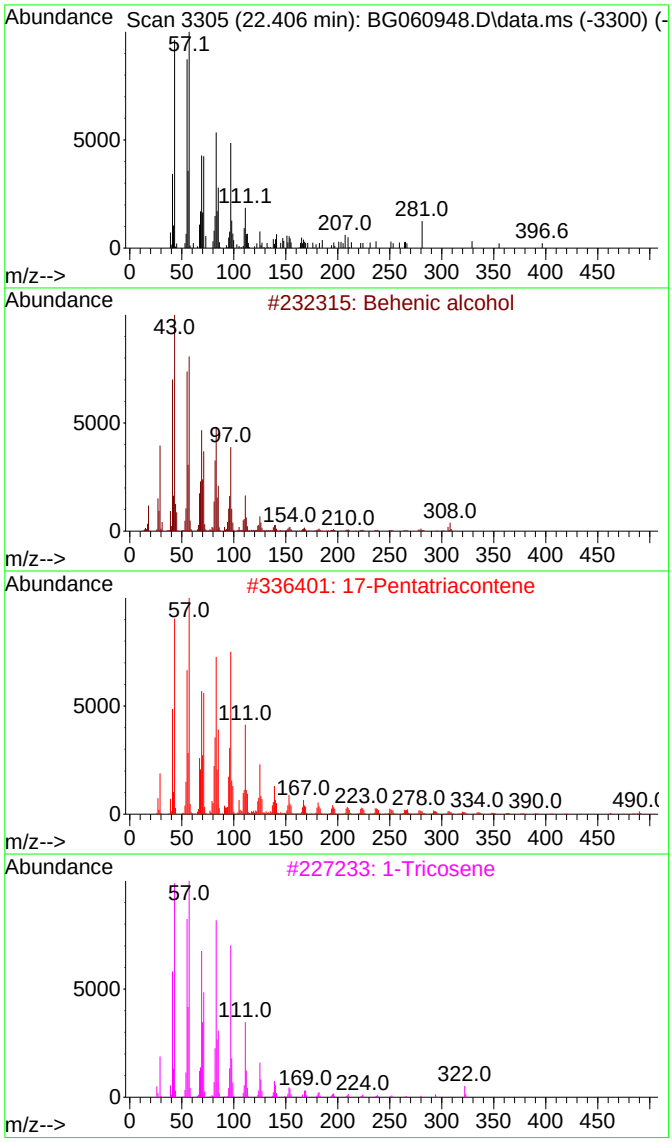
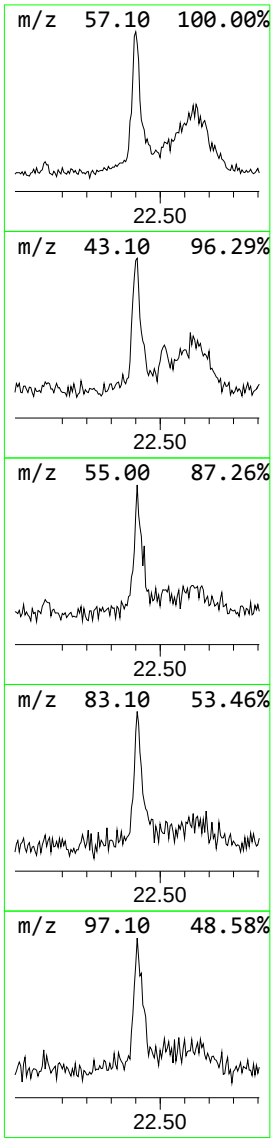
Peak Number 8 Behenic alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.406	2.47 ng	144668	Chrysene-d12	21.571

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	87
2	17-Pentatriacontene	491	C35H70	006971-40-0	86
3	1-Tricosene	322	C23H46	018835-32-0	80
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	80
5	9-Nonadecene	266	C19H38	031035-07-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060948.D
Acq On : 18 Apr 2024 23:21
Operator : MA/JU
Sample : P2124-02
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.158	8.6	ng	134957	1	7.940	313592	20.0
Propylene Glycol	3.675	11.9	ng	185888	1	7.940	313592	20.0
1-Phenoxypropan...	11.466	2.9	ng	61676	2	10.731	426712	20.0
unknown14.791	14.791	3.7	ng	133953	3	14.568	726146	20.0
n-Hexadecanoic ...	18.222	12.7	ng	664760	4	17.312	1048950	20.0
Octadecanoic acid	19.491	2.9	ng	169217	5	21.571	1172600	20.0
Cycloeicosane	21.242	9.2	ng	541767	5	21.571	1172600	20.0
Behenic alcohol	22.406	2.5	ng	144668	5	21.571	1172600	20.0